

2011.98722860

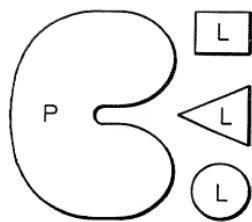


fig. 1A

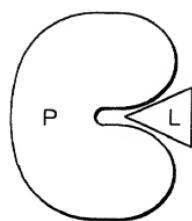


fig. 1B

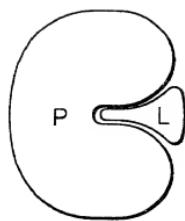


fig. 1C

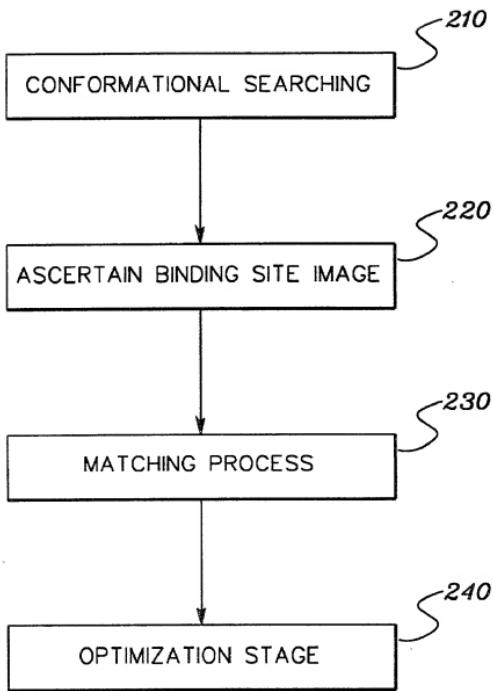


fig. 2

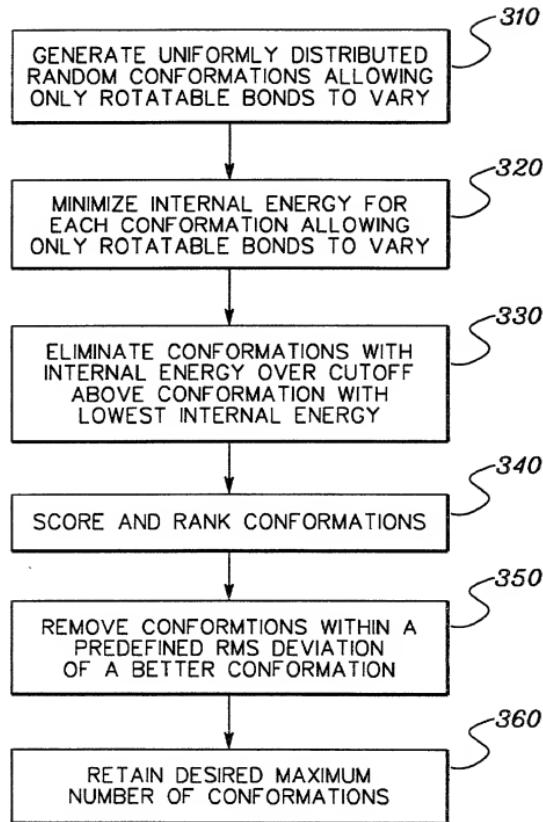


fig. 3

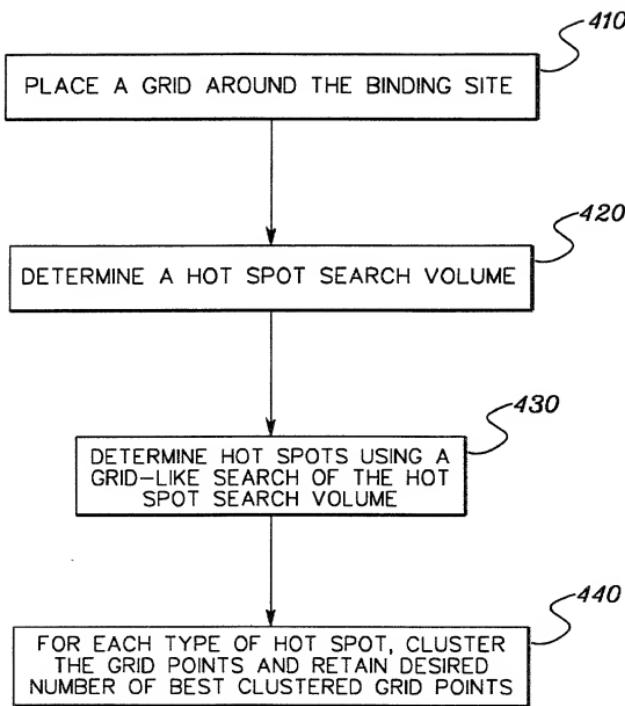


fig. 4

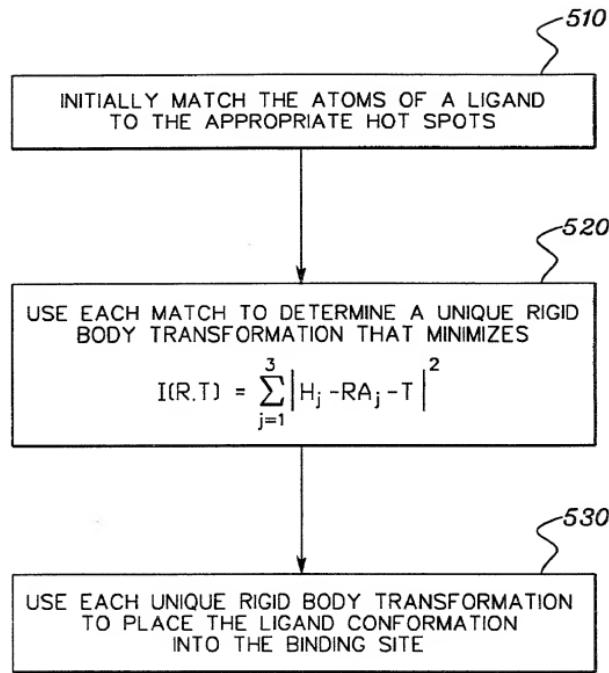


fig. 5

MATCHES FOR WHICH MORE THAN A
PREDETERMINED PERCENTAGE OF THE
LIGAND ATOMS HAVE A STERIC
CLASH ARE ELIMINATED

RANK REMAINING MATCHES USING
AN ATOM PAIRWISE SCORE, WITH A
DESIRED ATOM SCORE CUTOFF

AFTER RANKING, CLUSTER THE
MATCHES AND SELECT TOP N

OPTIMIZE EACH REMAINING MATCH
OF THE TOP N USING A BFCS
OPTIMIZATION ALGORITHM WITH
A SIMPLE ATOM PAIRWISE SCORE,
ALLOWING THE TRANSLATION,
ROTATION AND ROTATABLE
BONDS TO VARY

fig. 6

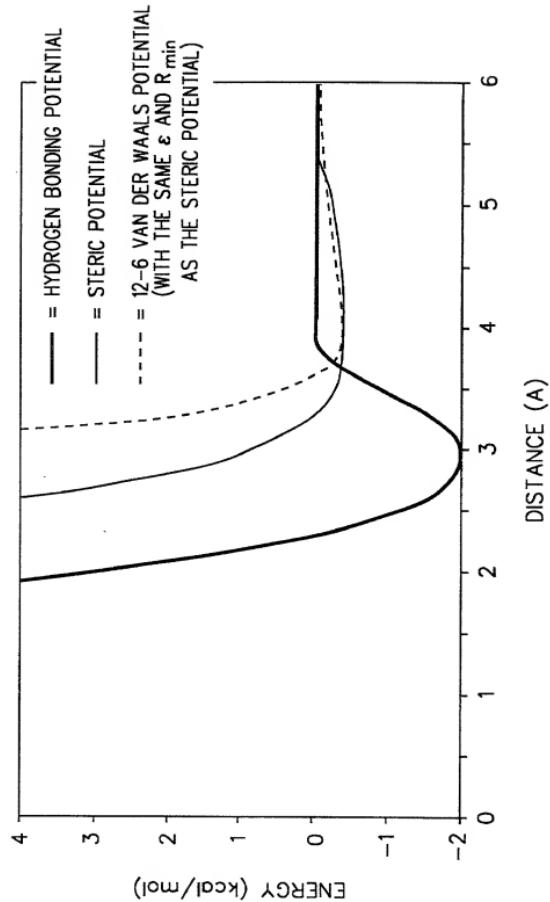


fig. 7

800

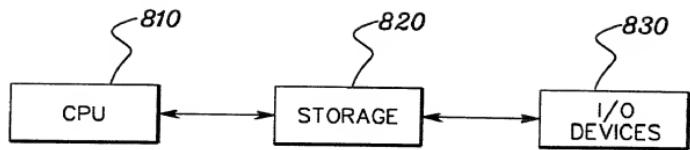


fig. 8

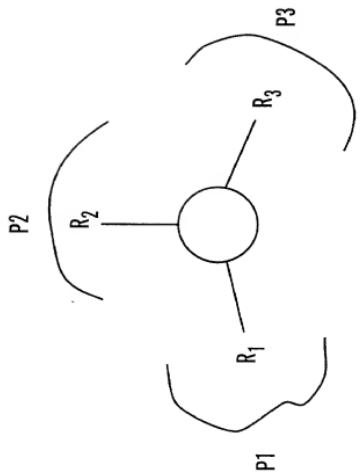


FIG. 9

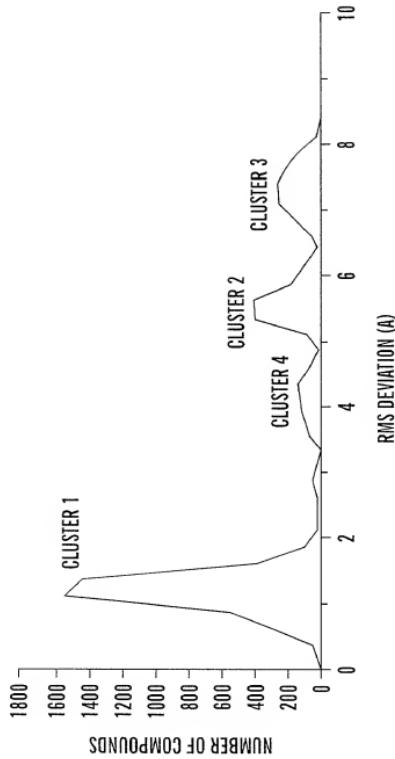


FIG. 10